**FINAL REPORT**
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# Lagrangian Simulation of Combustion
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**Principal Investigator: Prof. Ahmed F. Ghoniem**
**Massachusetts Institute of Technology**
**Department of Mechanical Engineering**
**Cambridge, MA 02139**

## 1. Objectives

A Lagrangian approach for the simulation of reactive flows has been developed during the course of this project [2, 3], and has been applied to a number of significant and challenging problems including the transverse jet simulations. An efficient strategy for parallel domain decomposition has also been developed to enable the implementation of the approach on massively parallel architecture. Since 2005, we focused our efforts on the development of a semi-Lagrangian treatment of diffusion, and fast and accurate Lagrangian simulation tools for multiphysics problems including combustion.

## 2. Accomplishments

### 2.1. Diffusion and Remeshing

Computational elements in Lagrangian vortex methods can be better understood by expressing them as measures or, more generally, distributions [11]. In this context, we developed an algorithm that allows us to treat diffusion and remeshing simultaneously. The strength of each computational element is interpolated on a Cartesian grid, and then each grid point containing nontrivial strength is converted into a particle. Interpolation kernels are obtained by utilizing the moment based redistribution method [12]. The resulting algorithm has been analyzed for consistency and convergence [ **1**], and it has been applied to several large-scale 3D vortex simulations [ **1**[ 5]. The scheme is $O(N)$, the computational cost of redistribution has thus been drastically decreased and the number of computational elements is now controlled by the grid size, enabling truly large-scale simulations.

### 2.2. Multi-Purpose Adaptive Tree Code

Lagrangian simulations require the evaluation of various $N$-body interactions, whose cost scales as $O(N^2)$, where $N$ is the number of computational elements. Direct summation is thus prohibitively expensive for the evaluation of these interactions, and one needs to employ hierarchical methods for fast summation, which limits the computational load roughly within $O(N \log N)$. Our multi-physics simulations require the computation of the vortical velocity and the expansion velocity, as well as their gradients. In the transport element method, there is also a need to recover the scalar field from its gradient. In previous years, we used a fast parallel tree-code to deal with the computations of the vortical velocity field [13]. Since all of the quantities of interest, i.e., the vortical velocity, the expansion velocity, their gradients and the scalar field, can be effectively computed from one single Taylor series expansion of a potential and a recombination of its Taylor coefficients, we extended this fast summation algorithm to all the operators needed in our simulations [ **5**]. Particle-particle interactions are now replaced by a smaller number of particle-cluster interactions, which can be efficiently computed from the Taylor coefficients. An extension of the current tree-code in which we use a low-order algebraic kernel to one in which one can use a high-order algebraic kernel has been implemented by Wee *et al.* [ **7**]. The use of a high-order algebraic kernel guarantees efficiency and better convergence characteristics. Tests were performed to check the algorithm's accuracy and efficiency [ **7**[ 9]. Finally, an efficient strategy for the parallelization of this multi-purpose adaptive tree-code has been developed utilizing a similar strategy as the one used in [ **3**].

## 2.3. Multi-Physics Simulations

### 2.3.1. From Filaments to Elements

Our first motivation for the development of a multi-purpose treecode was the transition from vortex filaments representation of the vorticity field [ **2**[ 3[ 8] to a vortex element representation [ **5**[ 9[10]. Filaments are practical for inviscid simulations because the maintain a solenoidal vortex field identically, but these geometric advantages are lost when we deal with diffusion [ **1**]. Moreover, their implementation is challenging since one must keep track of the connectivity between the vortex particles. The element based multi-purpose treecode [ **5**] allows us to compute the velocity gradients at each particle locations, so that the stretching and tilting term can be directly evaluated at the particle location, without any information on its neighbors. As a consequence, memory efficiency is improved and better flexibility is achieved.

### 2.3.2. Transport Element Methods

Another motivation for the development of the multi-purpose treecode was to perform more efficient simulations using the transport element method [ **5**]. In the transport element method, when solving a reactive transport problem of a scalar variable, one discretizes the gradient of the scalar field instead of discrediting the scalar field itself. The computational elements have thus a smaller support. Note that when using Boussinesq approximation, the computation of the baroclinic generation of vorticity only requires the knowledge of the scalar gradient, not the scalar itself. Moreover, the support of scalar gradients roughly coincides with that of vorticity in reacting flows, and we may use only one single set of elements to represent both. This is another advantage of the method which leads to a more efficient utilization of the computational elements. For highly reactive flows, this support is only a fraction of the computational domain, which makes the use of transport element methods very attractive for combustion simulations. Various convective heat transfer problems are solved for demonstrating the capabilities of the TEM. We investigated the evolution of a thermal sphere and the interactions of two thermal spheres under gravity and under different configuration in [ **5**].

### 2.3.3. Simulations of Transverse Jets

A viscous vortex code has been developed to study transverse jets under the influence of viscous diffusion. Several cases of transverse jets have been run with various jet-crossflow velocity ratio and jet Reynolds number. We have explored the impact of nozzle-edge vortical perturbations on the structure and evolution of an incompressible transverse jet at high Reynolds number [ **2**, [ **3**], the effect of viscosity on the jet, as well the effect of a no-slip wall boundary condition [ **8**]. In our previous implementations of the convection substep, we only cancelled the no-flow boundary condition, i.e., the impermeability of the solid wall, by having an image vorticity distribution during the computation of the velocity field. In the new implementation, we added a vorticity distribution at the wall to cancel the tangential velocity. Wee *et al.* [ **8**] provide a complete description of the vorticity generation mechanism and associated algorithms, and shows that the wall boundary layer separation is critical to understanding jet behaviors.

Finally, an application of the transport elements method to the transverse jet problem has been implemented in order to understand how buoyancy affects the jet vortical structures. The algorithm, as well as a comparison between a viscous and a buoyant jet simulation can be found in [ **5**].

### 2.3.4. Lagrangian Simulation of Combustion

We applied the transport elements method to the three-dimensional simulations of multi-physics problems, where the flow field and the scalar field are coupled by various two-way interaction mechanisms, i.e., baroclinicity, thermal expansion, and chemical reactions [ **9**]. The Schwab-Zeldovich formulation has been used to develop a diffusion-controlled combustion algorithm at Le = 1. This way, all the information on chemical reactions and temperature distribution can be recovered from a single scalar, i.e., the Schwab-Zeldovich variable, which is advected and diffused in its gradient form.
The newly implemented flow algorithm [ **9**] differs from the previous "buoyant flow" algorithm [ **5**] in two ways. The first being the addition of an expansion velocity during the convection step. Which augments the vortical velocity. This additional velocity comes from the temporal density change. The second difference is the limitation of the baroclinic generation to the first order for the reacting case [ **5**].

The serial combustion algorithm efficiency allow us to reach convergence in the case of methane spheres or rings with Gaussian distributions of fuel [ **9**]. However, the algorithm will be parallelized and used in our transverse jet simulations to investigate the impact of reaction on the jet structure.

## 3. Conclusion

We developed a fast algorithm for simultaneous treatment of diffusion and remeshing for 3D Lagrangian methods. We investigated the interaction between the wall boundary layer and the transverse jet. We showed that new vortical structures, i.e., near wall jet vortices created by the separation of the wall boundary layer, exert qualitative and quantitative impacts on the jet overall structure [ **8**].

The Transport Element Method has been used to investigate the buoyancy effects on the transverse jet problem [10]. The non-buoyant and buoyant cases were compared by giving a complete description of the flow fields. The combination of vortex methods, the TEM and our multipurpose adaptive treecode allow us to perform accurate and time efficient simulations of the jet. We are thus getting closer to the final objective, which is the fast and accurate simulation of a 3D reacting transverse jet.

## 4. Future Work

The present report suggests a number of avenues for future work, the first step being the development of the transverse reacting jet, for which the scalar gradient in the transverse jet code will simply be replaced by the gradient of the Schwab-Zeldovich variable. Our major concern for the reacting jet simulation is whether or not sufficient accuracy will be maintained during long time simulations. Secondly, it seems important to formulate a better model for the in-pipe flow structures. This upgrade would allow us to capture the hovering vortex structures in the pipe.

Many efforts have been made on elucidating the mechanisms underlying the formation of organized vortical structures in the near field and the subsequent breakdown of these structures into small scales for the non-buoyant inviscid and viscous case. Now, we have to understand how buoyancy and the expansion velocity will affect these vortical structures, how it will affect the mixing rate between the fluid coming from the jet and the ambient, and finally, how these additional effects will change the entrainment of the ambient fluid. We will also study the impact of the strong mixing due to the counter-rotating vortex pair on the flame structure, and attempt to control the heat release by modulating the jet.

## 5. Recent Publications

[ 1 ] D. Wee and A. F. Ghoniem, *Modified interpolation kernels for treating diffusion and remeshing in vortex methods*, Journal of Computational Physics 213 (2006) 293-263.

[ 2 ] Y. M. Marzouk and A. F. Ghoniem, *Actuating transverse jets via nozzle-edge vortical perturbations*, AIAA Technical Paper, AIAA 2006-1492 (2006).

[ 3 ] Y. M. Marzouk and A. F. Ghoniem, *Vorticity structure and evolution in a transverse jet*, Journal of Fluid Mechanics 575 , 2007, 267 - 305

[ 4 ] F. Schlegel, *A Fast 3D Particle Method for Simulations of Buoyant and Reacting Flows*, MS Thesis, Massachusetts Institute of Technology (2007).

[ 5 ] F. Schlegel, D. Wee, A. F. Ghoniem, *A fast 3D particle method for the simulation of buoyant flow,* J. Comput. Phys. *In Press, Corrected Proof, Available online 10 April 2008*

[ 6 ] D. Wee, PhD Thesis, *Lagrangian Simulation of Transverse Jets with a distribution-based Diffusion Scheme*, Massachusetts Institute of Technology, Cambridge, MA, 2007.

## 6. In Preparation for Publication

[ 7 ] D. Wee, Y. M. Marzouk and A. F. Ghoniem, *A tree-code algorithm for a high-order algebraic kernel in vortex methods*. Submitted for publication in SIAM Journal on Scientific Computing.

[ 8 ] D. Wee, Y. M. Marzouk and A. F. Ghoniem, *Vorticity transformations in a transverse jet at finite Reynolds number*. In preparation for publication in Journal of Fluid Mechanics.

[ 9 ] F. Schlegel, D. Wee, A. F. Ghoniem, *Lagrangian Simulation of Combustion*. In preparation for publication.

[10 ] F. Schlegel, D. Wee, A. F. Ghoniem, *Application of the Transport Element Method to the Buoyant Jet Problem*. In preparation for publication.

## 7. Other related references

[11 ] G. Friedlander & M. Joshi, *Introduction to the Theory of Distributions*, 2nd. ed., Cambridge University Press (1998).

[12 ] S. Shankar & L. van Dommelen, A new diffusion procedure for vortex methods, *Journal of Computational Physics* 127 (1996) 88-109.

[13 ] K. Lindsay and R. Krasny. *A particle method and adaptative treecode for vortex sheet motion in three-dimensional flow*. Journal of Computational Physics 172, 879-907(2001)